

Classifying superconductivity in an infinite-layer nickelate Nd_{0.8}Sr_{0.2}NiO₂

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ABSTRACT

Recently Li et al. (2019 Nature **572** 624) discovered a new type of oxide superconductor Nd_{0.8}Sr_{0.2}NiO₂ with $T_c = 14$ K. To classify superconductivity in this infinite-layer nickelate experimental upper critical field, $B_{c2}(T)$, and the self-field critical current densities, $J_c(sf, T)$, reported by Li et al. (2019 Nature **572** 624), are analysed in assumption of s -, d -, and p -wave pairing symmetries and single- and multiple-band superconductivity. Based on deduced the ground-state superconducting energy gap, $\Delta(0)$, the London penetration depth, $\lambda(0)$, the relative jump in electronic specific heat at T_c , $\Delta C/C$, and the ratio of $2\Delta(0)/k_B T_c$, we conclude that Nd_{0.8}Sr_{0.2}NiO₂ is type-II high- κ weak-coupled single-band s -wave superconductor.

Introduction

For several decades the term of infinite-layer superconductor was referred to a copper-oxide superconducting compounds, Sr_{1-x}M_xCuO₂ (M = La, Nd, Ca, Sr...) [1,2], until recently, Li et al. [3] have extended this class of unconventional superconductors by the discovery of superconductivity at $T_c = 14$ K in Nd_{0.8}Sr_{0.2}NiO₂ nickelate. Thus, bulk superconducting oxides family, i.e. tungsten bronzes [4], titanates [5], bismuthates [6], cuprates [7], and ruthenates [8] extends by a new nickelate member. Several research groups proposed different models for superconducting state in this compound [9–12], while the exhibiting of the superconducting state in this compound is in a debate [13].

In this paper, to classify superconductivity in this new class of oxide superconductors the temperature-dependent upper critical field, $B_{c2}(T)$, and the self-field critical current density, $J_c(sf, T)$, are analysed within s -, d -, and p -pairing symmetries. In result, it is shown that infinite-layer Nd_{0.8}Sr_{0.2}NiO₂ nickelate is weak-coupled single band s -wave superconductor.

Models description

The Ginzburg-Landau theory [14] has two fundamental lengths, one is the coherence length, $\xi(T)$, and the second is London penetration depth, $\lambda(T)$. The ground state coherence length, $\xi(0)$, is given by [14,15]:

$$B_{c2}(0) = \frac{\phi_0}{2 \cdot \pi \cdot \xi^2(0)} \quad (1)$$

where $\phi_0 = 2.068 \cdot 10^{-15}$ Wb is magnetic flux quantum, and $B_{c2}(0)$ is the ground state upper critical field. For temperature dependent coherence length, $\xi(T)$, several models were proposed [14,15–21]. In this paper, to deduce the ground state coherence length, $\xi(0)$, in infinite-layer Nd_{0.8}Sr_{0.2}NiO₂ nickelate superconductor, three models are used. The first model was proposed by Gor'kov [16,17] (Gor'kov model):

$$B_{c2}(T) = \frac{\phi_0}{2 \cdot \pi \cdot \xi^2(0)} \cdot \left(\frac{1.77 - 0.43 \cdot \left(\frac{T}{T_c}\right)^2 + 0.07 \cdot \left(\frac{T}{T_c}\right)^4}{1.77} \right) \cdot \left[1 - \left(\frac{T}{T_c}\right)^2 \right] \quad (2)$$

The second model was proposed by Baumgartner et al. [20] (B-WHH):

$$B_{c2}(T) = \frac{\phi_0}{2 \cdot \pi \cdot \xi^2(0)} \cdot \left(\frac{\left(1 - \frac{T}{T_c}\right) - 0.153 \cdot \left(1 - \frac{T}{T_c}\right)^2 - 0.152 \cdot \left(1 - \frac{T}{T_c}\right)^4}{0.693} \right) \quad (3)$$

And the third model was proposed recently in our recent report [21]:

$$B_{c2}(T) = \frac{\phi_0}{2 \cdot \pi \cdot \xi^2(0)} \cdot \left(\frac{1.77 - 0.43 \cdot \left(\frac{T}{T_c}\right)^2 + 0.07 \cdot \left(\frac{T}{T_c}\right)^4}{1.77} \right)^2 \cdot \frac{1}{1 - \frac{1}{2 \cdot k_B \cdot T} \cdot \int_0^\infty \frac{d\epsilon}{\cosh^2 \left(\frac{\sqrt{\epsilon^2 + \Delta^2(T)}}{2 \cdot k_B \cdot T} \right)}} \quad (4)$$

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where k_B is Boltzmann constant, and $\Delta(T)$ is the temperature-dependent superconducting gap, for which analytical expression was given by Gross et al. [22]:

$$\Delta(T) = \Delta(0) \cdot \tanh \left[\frac{\pi \cdot k_B \cdot T_c}{\Delta(0)} \cdot \sqrt{\eta \cdot \frac{\Delta C}{C} \cdot \left(\frac{T_c}{T} - 1 \right)} \right] \quad (5)$$

where $\Delta(0)$ is the ground state energy gap amplitude, $\Delta C/C$ is the relative jump in electronic specific heat at T_c , $\eta = 2/3$ for s -wave superconductors [22].

Thus, $\xi(0)$ and T_c can be obtained by fitting experimental $B_{c2}(T)$ data to Eqs. (2)–(4). In addition, $\Delta C/C$, $\Delta(0)$ and, thus, the ratio of $\frac{2\Delta(0)}{k_B T_c}$, can be deduced as free-fitting parameters by fitting experimental $B_{c2}(T)$ data to Eq. (4). More details about the procedures can be found elsewhere [23].

There is an alternative way to deduce $\Delta(0)$, $\Delta C/C$, T_c and $\frac{2\Delta(0)}{k_B T_c}$ by the fit of experimental self-field critical current density, $J_c(\text{sf}, T)$, to universal equation, which is for thin-film superconductors reduced to simple form [23,24]:

$$J_c(\text{sf}, T) = \frac{\phi_0}{4\pi\mu_0} \cdot \frac{\ln \left(1 + \sqrt{2} \cdot \frac{\lambda(0)}{\xi(0)} \right)}{\lambda^3(T)} \quad (6)$$

where $\mu_0 = 4\pi \times 10^{-7} \text{H/m}$ is the magnetic permeability of free space, and the London penetration depth, $\lambda(T)$, is given by:

$$\lambda(T) = \frac{\lambda(0)}{\sqrt{1 - \frac{1}{2 \cdot k_B \cdot T} \cdot \int_0^\infty \frac{d\varepsilon}{\cosh^2 \left(\frac{\sqrt{\varepsilon^2 + \Delta^2(T)}}{2 \cdot k_B \cdot T} \right)}}} \quad (7)$$

for s -wave superconductors, where $\Delta(T)$ is given by Eq. (5) [22,25].

$$\lambda(T) = \frac{\lambda(0)}{\sqrt{1 - \frac{1}{2 \cdot k_B \cdot T} \cdot \int_0^{2\pi} \cos^2(\theta) \cdot \left(\int_0^\infty \frac{d\varepsilon}{\cosh^2 \left(\frac{\sqrt{\varepsilon^2 + \Delta^2(T, \theta)}}{2 \cdot k_B \cdot T} \right)} \right) d\theta}} \quad (8)$$

for d -wave superconductors, where the superconducting energy gap, $\Delta(T, \theta)$, is given by [22,25]:

$$\Delta(T, \theta) = \Delta_m(T) \cdot \cos(2\theta) \quad (9)$$

where $\Delta_m(T)$ is the maximum amplitude of the k -dependent d -wave gap given by Eq. (5), θ is the angle around the Fermi surface subtended at (π, π) in the Brillouin zone (details can be found elsewhere [22,25,26]). In Eq. (9) the value of $\eta = 7/5$ [22,25,26].

1. And p -wave symmetry [22,25], which only recently was tested to fit critical current densities in superconductors [22,25]:

$$\lambda_{(p,a)(\perp, \parallel)}(T) = \frac{\lambda_{(p,a)(\perp, \parallel)}(0)}{\sqrt{1 - \frac{3}{4 \cdot k_B \cdot T} \cdot \int_0^\infty w_{\perp, \parallel}(x) \cdot \left(\int_0^\infty \frac{d\varepsilon}{\cosh^2 \left(\frac{\sqrt{\varepsilon^2 + \Delta_{p,a}^2(T) \cdot f_{p,a}^2(x)}}{2 \cdot k_B \cdot T} \right)} \right) dx}} \quad (10)$$

where subscripts p , a , \perp , and \parallel designate polar, axial, perpendicular and parallel cases respectively. For this symmetry, the gap function is given by [22,25]:

$$\Delta(\hat{k}, T) = \Delta(T) \cdot f(\hat{k}, \hat{l}) \quad (11)$$

where, $\Delta(T)$ is the superconducting gap amplitude, \mathbf{k} is the wave vector, and \mathbf{l} is the gap axis. Thus, temperature dependence of $\lambda(T)$ is determined by mutual orientation of the vector potential, \mathbf{A} , and the gap axis, \mathbf{l} , which is for transport current experiment just the orientation of the crystallographic axes of the film compared with the direction of the electric current. There are two distinctive orientations, $\mathbf{A} \parallel \mathbf{l}$ (when \mathbf{A} is

perpendicular to \mathbf{l}) and polar $\mathbf{A} \parallel \mathbf{l}$ (when \mathbf{A} is parallel to \mathbf{l}) [22,25]. More details can be found elsewhere [22,25,26]). The function of $w_{\perp, \parallel}(x)$ in Eq. (10) is:

$$w_{\perp}(x) = (1 - x^2)/2 \quad (12)$$

and

$$w_{\parallel}(x) = x^2 \quad (13)$$

and the gap amplitude in Eq. (11) is just Eq. (5), but η is given by [25]:

$$\eta_{p,a} = \frac{2}{3} \cdot \frac{1}{\int_0^1 f_{p,a}^2(x) \cdot dx} \quad (14)$$

where

$$f_p(x) = x; \text{ polar configuration} \quad (15)$$

$$f_a(x) = \sqrt{1 - x^2}; \text{ axial configuration} \quad (16)$$

More details about the $J_c(\text{sf}, T)$ analysis for p -wave symmetry can be found elsewhere [26,27].

By substituting Eqs. (5), (7)–(13) in Eq. (6), one can fit experimental $J_c(\text{sf}, T)$ data to s -, d -, p -wave gap symmetries to deduce $\lambda(0)$, $\Delta(0)$, $\Delta C/C$, T_c and $\frac{2\Delta(0)}{k_B T_c}$ as free-fitting parameters. This approach is recently applied for wide range of thin film unconventional superconductors [23,24,26–32].

$B_{c2}(T)$ analysis

There are several criteria to define $B_{c2}(T)$ from experimental $R(T)$ curves. In this paper to define $B_{c2}(T)$ we use the criterion of 3% of normal state resistance, $R_{\text{norm}}(T)$, for $R(T)$ curves of $\text{Nd}_{0.8}\text{Sr}_{0.2}\text{NiO}_2$ presented in Fig. 4 (a) by Li et al. [3]. The fits of $B_{c2}(T)$ data to three models are shown in Fig. 1. It can be seen that $\xi(0)$ values deduced by three models are close to each other and following analysis of $J_c(\text{sf}, T)$ will be utilized an average value of:

$$\xi(0) = 5.7 \pm 0.3 \text{ nm} \quad (17)$$

This deduced value for $\xi(0)$ is in reasonable agreement with $\xi(0) = 4.5 \text{ nm}$ reported by Jovanović et al. [33] for copper-oxide-based infinite layer counterpart of $\text{La}_{1-x}\text{Sr}_x\text{CuO}_2$.

Deduced values by the fit to Eq. (4):

$$\frac{2\Delta(0)}{k_B T_c} = 3.5 \pm 0.3 \quad (18)$$

$$\frac{\Delta C}{C} = 1.5 \pm 0.2 \quad (19)$$

are, within uncertainties, equal to BCS [34] weak-coupling limits of 3.53 and 1.43 respectively, and the former deduced value is equal to recently deduced value of:

$$\frac{2\Delta(0)}{k_B T_c} = 3.51 \pm 0.05 \quad (20)$$

for s -wave oxide superconductor of $\text{Ba}_{0.51}\text{K}_{0.49}\text{BiO}_3$ [35].

It should be noted that there is no sign in experimental $B_{c2}(T)$ data that $\text{Nd}_{0.8}\text{Sr}_{0.2}\text{NiO}_2$ exhibits two superconducting band state, which can be seen as sharp enhancement in amplitude of $B_{c2}(T)$ at critical temperature of the second superconducting band opening (see for details Ref. 36).

$J_c(\text{sf}, T)$ analysis

The critical current density, J_c , is defined as the lowest, detectable in experiment, value of electric power dissipation in a superconductor on electric current flow. For available $E(I)$ curves presented by Li et al. [3] in their Fig. 3(f), the critical current density at self-field condition

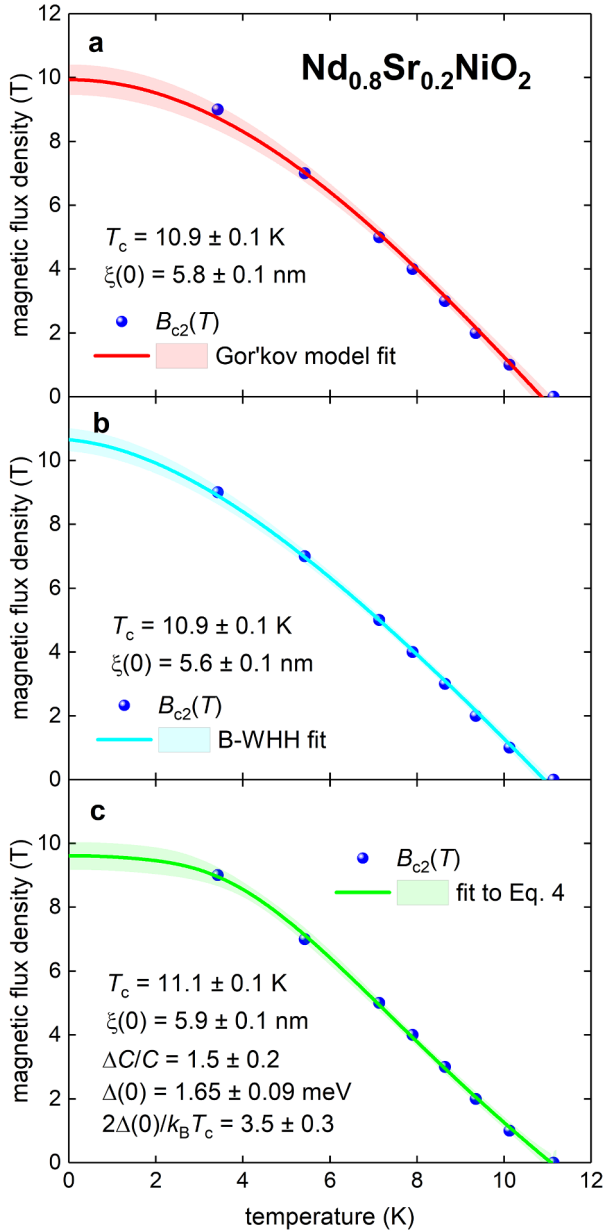


Fig. 1. The upper critical field, $B_{c2}(T)$, of $\text{Nd}_{0.8}\text{Sr}_{0.2}\text{NiO}_2$ (reported by Li et al. [3]) and data fits to three models (Eqs. (2)–(4)). (a) Fit to Gor'kov model, the fit quality is $R = 0.995$. (b) Fit to B-WHH, $R = 0.998$. (c) Fit to Eq. (4), $R = 0.9993$. 95% confidence bars are shown.

(when no external magnetic field is applied), $J_c(\text{sf}, T)$, can be defined at the lowest value of electric field of $E_c = 3 \text{ V/cm}$. Experimental $J_c(\text{sf}, T)$ deduced by this E_c criterion and the fit to single band s -wave model (i.e., Eqs. (6) and (7) for which $\xi(0) = 5.7 \text{ nm}$ was fixed) are shown in Fig. 2(a). It can be seen that the fit is excellent, and deduced superconducting parameters (Fig. 2(a) and Table 1) are within BCS weak-coupling limits.

Deduced $\lambda(0) = 740 \pm 3 \text{ nm}$ is similar to $\lambda(0) = 690\text{--}850 \text{ nm}$ measured for samples possessing maximal T_c values for cuprate counterpart $\text{La}_{1-x}\text{Sr}_x\text{CuO}_2$ [37].

By utilizing deduced $\lambda(0)$ value the Ginzburg-Landau parameter $\kappa = \frac{\lambda(0)}{\xi(0)} = 130$ which is similar to $\text{La}_{1-x}\text{Sr}_x\text{CuO}_2$ [33,37] and this value is at the upper-level range for other cuprates and unconventional superconductors [15,23,24,26,38–43].

Alternatively, d - and p -wave superconducting gap symmetries can be considered. The fits to d -wave symmetry, as well as to polar $A||I$ and

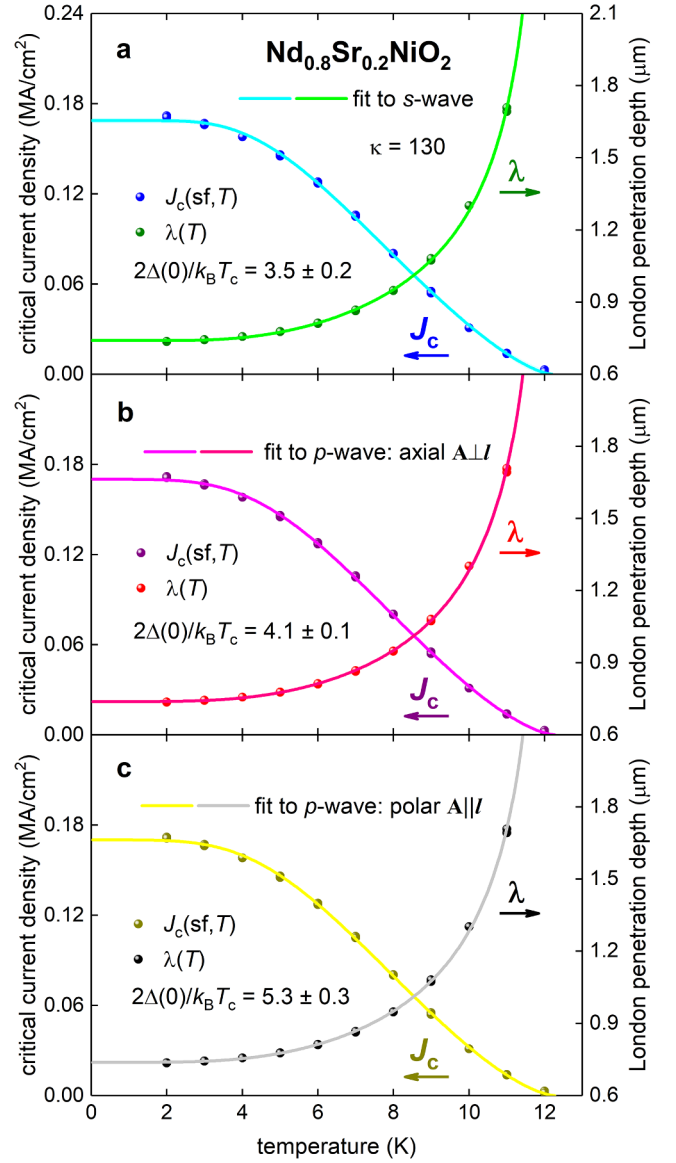


Fig. 2. The self-field critical current density, $J_c(\text{sf}, T)$, for $\text{Nd}_{0.8}\text{Sr}_{0.2}\text{NiO}_2$ thin film with raw data processed from the work of Li et al. [3] and data fits to three single-band models for which deduced parameters are close to weak-coupling BCS limits. For all models $\xi(0) = 5.7 \text{ nm}$ was used. (a) s -wave fit, $\lambda(0) = 740 \pm 3 \text{ nm}$, $T_c = 12.2 \pm 0.1 \text{ K}$, the goodness of fit $R = 0.995$; (b) p -wave axial $A\perp I$ fit, $\lambda(0) = 738 \pm 2 \text{ nm}$, $T_c = 12.3 \pm 0.1 \text{ K}$, $R = 0.997$; (c) p -wave polar $A||I$ fit, $\lambda(0) = 735 \pm 2 \text{ nm}$, $T_c = 12.4 \pm 0.1 \text{ K}$, $R = 0.9990$. Other deduced parameters are listed in Table 1.

axial $A||I$ of p -wave are shown in Fig. 3. However, fits to these symmetries reveal very large $\frac{2\Delta(0)}{k_B T_c}$ values (Table 1 and Fig. 3). And based on this, these three symmetries can be excluded from further consideration.

The cases of polar $A||I$ and axial $A\perp I$ gap symmetries are still hypothetically possible (Table 1), and $J_c(\text{sf}, T)$ fits to these models are shown in Fig. 2(b, c) respectively, however, for given experimental conditions (i.e. epitaxial c -axis oriented thin film) expected geometry is polar $A\perp I$ [21], but for this geometry deduced $\frac{2\Delta(0)}{k_B T_c} \cong 1950$ (Fig. 3(c)) which does not have physical meaningful value.

It should be stressed that there is no sign for two-band superconductivity in $\text{Nd}_{0.8}\text{Sr}_{0.2}\text{NiO}_2$ which usually can be detected by a sharp enhancement in $B_{c2}(T)$ and $J_c(\text{sf}, T)$ at critical temperature of the second band opening [24,36].

It is important to note that there are strong experimental evidences [44] that cuprate infinite layer superconductor, $\text{Sr}_{0.90}\text{La}_{0.10}\text{CuO}_2$, which

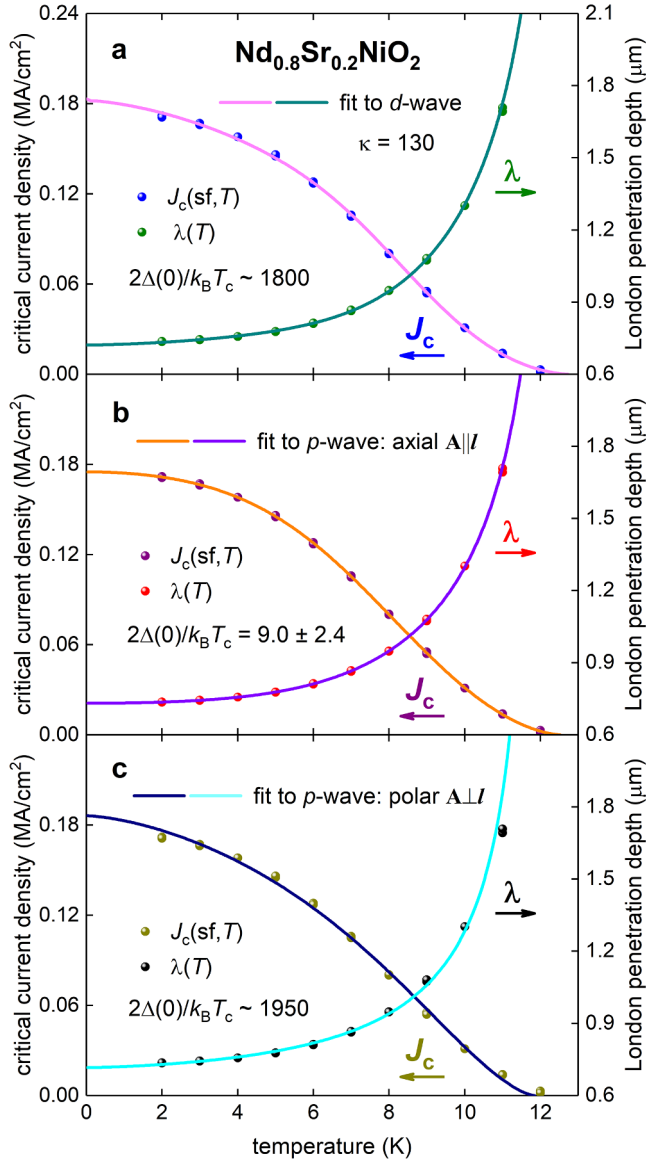


Fig. 3. The self-field critical current density, $J_c(sf, T)$, for $\text{Nd}_{0.8}\text{Sr}_{0.2}\text{NiO}_2$ thin film with raw data processed from the work of Li et al. [3] and data fit to three single-band models for which deduced parameters are very different from weak-coupling BCS limits. Ground state superconducting coherence length of $\xi(0) = 5.7$ nm was used. (a) d -wave fit, $\lambda(0) = 721 \pm 4$ nm, $T_c = 12.7 \pm 0.2$ K, the goodness of fit $R = 0.997$; (b) p -wave axial $A_{||}I$ fit, $\lambda(0) = 738 \pm 2$ nm, $T_c = 12.53 \pm 0.05$ K, $R = 0.9996$; (c) p -wave polar $A_{\perp}I$ fit, $\lambda(0) = 716 \pm 12$ nm, $T_c = 11.9 \pm 0.2$ K, $R = 0.986$. Other deduced parameters are listed in Table 1.

is perhaps the closest structural counterpart of $\text{Nd}_{0.8}\text{Sr}_{0.2}\text{NiO}_2$ in the cuprate superconductors family [1,2,7,45,46] is s -wave superconductor [44]. In this regard, our finding that $\text{Nd}_{0.8}\text{Sr}_{0.2}\text{NiO}_2$ is s -wave superconductor is rather convincing, because it shows a similarity with cuprate superconductors, rather than to be a contradiction with cuprate superconductors, where d -wave superconductivity exhibits in materials with charge reservoir atomic layers.

To further demonstrate that available experimental data for $\text{Nd}_{0.8}\text{Sr}_{0.2}\text{NiO}_2$ superconductor is inconsistent with d -wave gap symmetry in Fig. 4 we show the fit of $J_c(sf, T)$ to d -wave model for which the ratio of $\frac{2\Delta(0)}{k_B T_c}$ was fixed to three different values: (a) to the weak-coupling limit, $\frac{2\Delta(0)}{k_B T_c} = 4.28$ [25,47], of d -wave superconductors (Fig. 4a); (b) to $\frac{2\Delta(0)}{k_B T_c} = 6.0$ which can be considered as very strong-coupling case

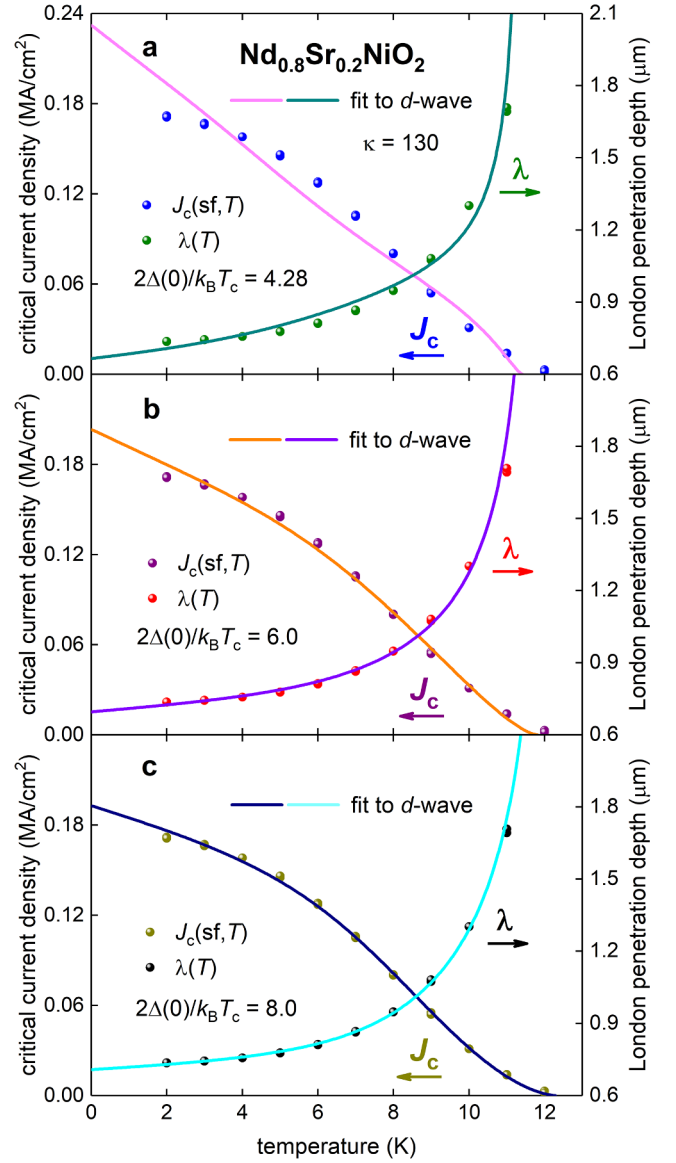


Fig. 4. The self-field critical current density, $J_c(sf, T)$, for $\text{Nd}_{0.8}\text{Sr}_{0.2}\text{NiO}_2$ thin film with raw data processed from the work of Li et al. [3] and data fit to single-band d -wave model with three fixed $\frac{2\Delta(0)}{k_B T_c}$ ratios. Ginzburg-Landau parameter $\kappa = 130$ is used for all three fits. (a) $\frac{2\Delta(0)}{k_B T_c} = 4.28$ (fixed), $\Delta C/C = 3.2 \pm 1.8$; $\lambda(0) = 665 \pm 5$ nm, $T_c = 11.4$ K, the goodness of fit $R = 0.854$; (b) $\frac{2\Delta(0)}{k_B T_c} = 6.0$ (fixed), $\Delta C/C = 1.5 \pm 0.2$; $\lambda(0) = 695 \pm 2$ nm, $T_c = 11.8$ K, the goodness of fit $R = 0.981$; (c) $\frac{2\Delta(0)}{k_B T_c} = 8.0$ (fixed), $\Delta C/C = 0.97 \pm 0.07$; $\lambda(0) = 708 \pm 1$ nm, $T_c = 12.3$ K, the goodness of fit $R = 0.994$.

of d -wave superconductivity; and (c) to $\frac{2\Delta(0)}{k_B T_c} = 8.0$ which was chosen to be overwhelmingly large. It can be seen in Fig. 4 that for all fits are not consistent with experimental $J_c(sf, T)$ data. Obviously that fit to d -wave pairing symmetry showed in Fig. 3(a) is better matched experimental data, but deduced free-fitting ratio of $\frac{2\Delta(0)}{k_B T_c} \approx 1800$ cannot be considered to have physical meaning as we mentioned already above.

By taking in account a good agreement between $\frac{2\Delta(0)}{k_B T_c}$ and $\frac{\Delta C}{C}$ values deduced from experimental $B_{c2}(T)$ and $J_c(sf, T)$ data for $\text{Nd}_{0.8}\text{Sr}_{0.2}\text{NiO}_2$ in the assumption of s -wave symmetry (Eqs. (18) and (19) and Table 1, respectively), which all are within BCS weak-coupling limits for this symmetry, and a fact that s -wave pairing symmetry is the most conventional symmetry we can conclude that $\text{Nd}_{0.8}\text{Sr}_{0.2}\text{NiO}_2$ nickelate is weak-coupling single band high- κ s -wave superconductor.

Table 1

Deduced $2\Delta(0)/k_B T_c$ and $\Delta C/C$ values for $\text{Nd}_{0.8}\text{Sr}_{0.2}\text{NiO}_2$ from $J_c(\text{sf}, T)$ fits to Eqs. (6)–(8) and BCS weak-coupling limits for the same parameters within for s -, d -, and p -wave pairing symmetries [20,23]. For d -wave symmetry, $\Delta_m(0)$ was used (which is the maximum amplitude of the k -dependent d -wave gap, $\Delta(\theta) = \Delta_m(0)\cos(2\theta)$).

Pairing symmetry and experiment geometry	Deduced $\frac{2\Delta(0)}{k_B T_c}$	BCS weak-coupling limit of $\frac{2\Delta(0)}{k_B T_c}$	Deduced $\frac{\Delta C}{C}$	BCS weak-coupling limit of $\frac{\Delta C}{C}$
s -wave	3.5 ± 0.2	3.53	1.5 ± 0.2	1.43
d -wave	$1.8 \cdot 10^3$	4.28	0.68 ± 0.08	0.995
p -wave; axial $A l$	4.1 ± 0.1	4.06	1.07 ± 0.08	1.19
p -wave; axial $A l$	9.0 ± 2.4	4.06	1.55 ± 0.05	1.19
p -wave; polar $A \perp l$	$1.95 \cdot 10^3$	4.92	2.5 ± 0.4	0.79
p -wave; polar $A l$	5.3 ± 0.3	4.92	0.63 ± 0.03	0.79

Conclusions

Recently discovered [3] an infinite-layer nickelate $\text{Nd}_{0.8}\text{Sr}_{0.2}\text{NiO}_2$ superconductor is a new member of bulk oxide superconductors for which experimental $B_{c2}(T)$ and $J_c(\text{sf}, T)$ data are analysed in this paper.

In result, it is found that an infinite-layer nickelate $\text{Nd}_{0.8}\text{Sr}_{0.2}\text{NiO}_2$ is weak-coupling single band high- κ s -wave superconductor.

Declaration of Competing Interest

The author declares that he has no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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